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NUCLEAR MAGNETIC RESONANCE METHODS FOR IDENTIFYING SITES IN PAPILLOMAVIRUS E2 PROTEIN

This application claims the benefit of U.S. Provisional Application Serial Nos. 60/197,459, filed 17 April 2000, 60/211,055, filed 13 June 2000, and 60/268,444 filed 13 February 2001, which are incorporated herein by reference in their entireties.

BACKGROUND OF THE INVENTION

An important aspect in understanding the function of biochemical processes is the elucidation of the nature of the associations between various species including, for example, the associations between ligands and proteins. Such associations may be non-covalent, wherein juxtapositions are energetically favored by hydrogen bonding, van der Waals forces, or electrostatic interactions, or they may be covalent. When physical binding is being studied, a target molecule is typically exposed to one or more compounds suspected of being ligands, and assays are then performed to determine if complexes between the target molecule and one or more of those compounds are formed. Such assays, as are well known in the art, test for gross changes (e.g., size, charge, and mobility) in the target molecule that indicate complex formation.

Where functional changes are measured, assay conditions are established that allow for measurement of biological or chemical events related to the target molecule (e.g., enzyme catalyzed reaction and receptor-mediated enzyme activation). To identify an alteration, the function of the target molecule is determined before and after exposure to the test compounds.

Assays involving the use of nuclear magnetic resonance (NMR) techniques are also known. NMR techniques may be used, for example, in conjunction with other assay methods to assess hits identified from physical binding screens or functional assay screens. If ¹H, ¹³C, and/or ¹⁵N resonance assignments are known for the target as well as either a solution or X-ray crystallographic structure, then the binding site location of identified ligands can be determined using NMR techniques.

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As such, definitive resonance assignments of the target are required as a first step. A DNA-binding protein, E2, which is encoded by the papillomavirus and is involved in transcriptional regulation and viral replication, is one such target.

SUMMARY OF THE INVENTION

In one aspect, the present invention provides a nuclear magnetic resonance method for identifying a site in a DNA-binding and dimerization domain of a papillomavirus E2 protein. In one embodiment, the method includes providing a first set of chemical shifts for atoms of a mixture including a ligand and the papillomavirus E2 protein, comparing the first set of chemical shifts to a second set of chemical shifts as listed in Table 1, and identifying at least a portion of the atoms that exhibit changes in chemical shifts, wherein the site includes the identified atoms. Preferably providing the first set of chemical shifts includes providing a mixture of the ligand and the papillomavirus E2 protein, allowing the ligand to interact with the papillomavirus E2 protein, obtaining a nuclear magnetic resonance spectrum of the mixture, and measuring chemical shifts of atoms from the spectrum. Preferably allowing the ligand to interact includes allowing the ligand and the protein to reach a binding equilibrium. Preferably the site is a ligand binding site. Preferably the papillomavirus E2 protein is encoded by the HPV-18 strain.

In another embodiment, the method includes providing a first $^{1}\text{H}^{-15}\text{N}$ heteronuclear single quantum correlation spectrum of a mixture including a ligand and the papillomavirus E2 protein, comparing the first $^{1}\text{H}^{-15}\text{N}$ heteronuclear single quantum correlation spectrum to a second $^{1}\text{H}^{-15}\text{N}$ heteronuclear single quantum correlation spectrum as illustrated in Figure 2, and identifying at least a portion of the amino acids having atoms that exhibit changes in chemical shifts, wherein the site includes the identified amino acids. Preferably providing the first spectrum includes providing a mixture of the ligand and the papillomavirus E2 protein, allowing the ligand to interact with the papillomavirus E2 protein, and obtaining a $^{1}\text{H}^{-15}\text{N}$ heteronuclear single quantum correlation spectrum of the mixture.

30 Preferably allowing the ligand to interact includes allowing the ligand and the

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protein to reach a binding equilibrium. Preferably the site is a ligand binding site. Preferably the papillomavirus E2 protein is encoded by the HPV-18 strain.

In another aspect, the present invention provides a machine-readable data storage medium including a data storage material encoded with nuclear magnetic resonance chemical shifts as listed in Table 1, wherein when a first set of chemical shifts is provided, the chemical shifts encoded on the data storage material are capable of being read by the machine to create a second set of chemical shifts, and the machine having programmed instructions that are capable of causing the machine to compare the first and second sets of chemical shifts to arrive at structural information.

In another aspect, the present invention provides a computer-assisted method for identifying a ligand binding site in a DNA-binding and dimerization domain of a papillomavirus E2 protein. The method includes providing a first set of nuclear magnetic resonance chemical shifts for atoms of a mixture including the ligand and the papillomavirus E2 protein, causing the first set of chemical shifts to be entered into memory of a computer, causing the computer to read a second set of chemical shifts as listed in Table 1 from a machine-readable data storage medium, causing the computer to compare the first and second sets of chemical shifts, and causing the computer to identify at least a portion of the atoms that exhibit changes in chemical shifts, wherein the ligand binding site includes the identified atoms. Preferably the papillomavirus E2 protein is encoded by the HPV-18 strain. Preferably the method further includes causing the computer to visually display a spatial arrangement of atoms of the ligand binding site.

Methods disclosed in the present invention for identifying sites offer advantages over other methods known in the art. For example, the present invention preferably provides methods for efficiently identifying binding sites for a wide range of chemically and physically diverse potential ligands.

The term "binding" as used herein, refers to a condition of proximity between a chemical entity or compound, or portions thereof, and the target protein or portions thereof. The association may be non-covalent, wherein the juxtaposition

is energetically favored by hydrogen bonding, van der Waals forces, or electrostatic interactions, or it may be covalent. The association may be a static interaction, or an equilibrium may be reached between associated and non-associated species. Preferably, a ligand that binds to a ligand binding site in a DNA-binding and dimerization domain of a papillomavirus E2 protein would also be expected to bind to or interfere with another ligand binding site whose structure defines a shape that falls within an acceptable error.

The term "ligand" as used herein means any chemical entity, compound, or portion thereof, that is capable of binding to a protein.

The term "change in chemical shifts" as used herein means the observation of an increase or decrease in chemical shift for a resonance, an increase or decrease in intensity for a resonance, or the failure to observe a resonance when comparing a resonance of an atom from the spectrum of a mixture of ligand and protein to the resonance of the same atom from the spectrum of the protein without the ligand

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is an illustration of the deviations from random coil chemical shifts of $^{13}C_{\alpha}$ resonances (in parts per million (ppm)) with assignments for the DNA-binding and dimerization domain of papillomavirus (strain HPV-18) E2 protein as a function of residue number. Random coil chemical shift values are from Wishart et al., Biochem. Cell Biol., 76:153-63 (1998). Locations of secondary structure according to the X-ray structure of BPV-1, HPV-16 and HPV-31 are shown with α (α -helix) and β (β -sheet).

Figure 2 is an illustration of the 2-dimensional ¹H-¹⁵N heteronuclear single quantum correlation spectrum with assignments for the DNA-binding and dimerization domain of a 0.84 mM papillomavirus (strain HPV-18) E2 protein at 300°K.

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DETAILED DESCRIPTION

Papillomaviruses are a diverse group of small DNA viruses that infect epithelial cells and cause tumor formation. All of the papillomaviruses encode a DNA-binding protein, E2, that is involved in transcriptional regulation and viral replication. E2 protein consists of a C-terminal DNA-binding and dimerization domain (E2-DBD) and N-terminal transactivation domain, separated by a flexible region. E2-DBD from bovine papillomavirus-1 (BPV-1) has been extensively studied, and the X-ray crystallographic structure of E2-DBD bound to DNA consists of a homodimer that includes an eight-stranded β-barrel and two pairs of α-helices (Hedge et al., Nature, 359:505-12 (1992)). The solution and/or crystal structures of homologous E2-DBDs from human papillomavirus-31 (HPV-31) (Liang et al., Biochemistry, 35:2095-2103 (1996), Bussiere et al., Acta Cryst., D54:1367-76 (1998)) and HPV-16 (Hedge et al., J. Mol. Biol., 284:1479-89 (1998)) have been reported and are similar to BPV-1.

The present invention preferably relates to the E2-DBD from the high risk strain HPV-18. The E2 protein of HPV-18 represses the expression of the major viral transforming genes E6 and E7 and is a cofactor for the replication protein E1 binding to the origin (Kasukawa et al., <u>J. Virol.</u>, 72:8166-73 (1998)). The pivotal role of E2 in transcriptional regulation and viral replication makes it a potential target for antiviral therapy.

E2-DBD of HPV-18 has 55% and 60% sequence identity to HPV-16 and HPV-31, respectively, and binds to the ACCN₆GGT recognition sequence. Preferably, two amino acid sequences are compared using the Blastp program, version 2.0.9, of the BLAST 2 search algorithm, as described by Tatusova et al., FEMS Microbiol Lett 174, 247-50 (1999), and available at http://www.ncbi.nlm.nih.gov/gorf/bl2.html. Preferably, the default values for all BLAST 2 search parameters are used, including matrix = BLOSUM62; open gap penalty = 11, extension gap penalty = 1, gap x_dropoff = 50, expect = 10, wordsize = 3, and filter on. In the comparison of two amino acid sequences using the BLAST search algorithm, structural similarity is referred to as "identity."

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The present invention provides a papillomavirus HPV-18 strain E2 protein DNA-binding domain having the ¹H-¹⁵N heteronuclear single quantum correlation spectrum shown in Figure 2. Each correlation is labeled as to the residue in the protein from which it arises if that has been determined. The process used to make the assignments is described in the examples. The chemical shifts of all assigned ¹H, ¹³C, and ¹⁵N resonances are listed in Table 1. The resonance assignments presented here provide the basis for determining sites, preferably binding site locations of ligands previously identified by other means. Chemical shift changes induced by addition of ligand to the protein sample are manifested by changes in the appearance of ¹H-¹⁵N HSQC spectra. Correlations that experience the largest ligand-induced chemical shift changes are preferably located near the ligand's binding site. To determine chemical shift changes, the protein ¹H, ¹³C, and ¹⁵N resonances are preferably assigned as extensively as possible.

Preferably, ligand binding sites include identified atoms that exhibit changes in chemical shifts. Preferably the identified atoms include at least one proton that, upon addition of ligand to the protein, either exhibits a change in ¹H chemical shift of at least about 0.04 ppm or is no longer observed. Preferably the identified atoms includes at least one carbon atom that, upon addition of ligand to the protein, either exhibits a change in ¹³C chemical shift of at least about 0.2 ppm or is no longer observed. Preferably the identified atoms include at least one nitrogen atom that, upon addition of ligand to the protein, either exhibits a change in ¹⁵N chemical shift of at least about 0.2 ppm or is no longer observed.

In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

EXAMPLES

The HPV-18 E2 protein consists of 410 amino acids with the DBD residing at the C-terminus (amino acids #329-410). E2-DBD cloning procedures resulted in the addition of methionine before amino acid 329 and six histidine residues after

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amino acid 410. Amino acid sequencing indicated that the N-terminal des-Met form of the E2-DBD protein was the major species produced.

E2-DBD was over-expressed in BL21 (DE3) E. coli cells using the pSRtac vector. Isotopically labeled samples were prepared in M9 glucose media containing ¹⁵NH₄Cl and unlabeled or U-¹³C-glucose. Cell pellets were lysed with intermittent mechanical disruption with a Tissuemizer (Tekmar Co., Cincinatti, OH). Clarified cell lysates were passed over Ni²⁺-NTA agarose (Qiagen, Inc., Valencia, CA), and further purified using Source 30Q anion exchange chromatography (Amersham Pharmacia Biotech, Inc.; Piscataway, NJ). The resulting E2-DBD exists as a homodimer of molecular weight 20.6 kDa under the conditions used for the NMR experiments.

The NMR samples typically consisted of 0.8 mM protein in buffer containing 20 mM phosphate, 50 mM NaCl, and 1 mM [²H₁₀] dithiothreitol (DTT) at pH 6.5 in 90% ¹H₂O/10% ²H₂O by volume. All NMR spectra were recorded at 27°C on a Bruker DRX-600 spectrometer (BRUKER NMR, Rheinstetten, Germany) using a 5 mm triple-resonance probe with 3-axis gradients. HNC $_{\alpha}$, HN(CO)C $_{\alpha}$, $C_{\beta}C_{\alpha}(CO)NH$, $H_{\beta}H_{\alpha}(CO)NH$, HNCO and HCCH-total correlation spectroscopy (HCCH-TOCSY) (mixing times 16 and 23 milliseconds) data sets were acquired using gradient-enhanced versions of the pulse sequences. Two-dimensional ¹H-¹⁵N Heteronuclear Single Quantum Correlation (HSQC) and ¹⁵N edited Nuclear 20 Overhauser Effect Spectroscopy-HSQC (NOESY-HSQC) (mixing time 80 milliseconds) spectra were also acquired. Proton chemical shifts were referenced to the ${}^{1}\text{H}_{2}\text{O}$ signal at 4.70 parts per million (ppm) (tetramethylsilane (TMS) = 0 ppm). The ¹⁵N and ¹³C chemical shifts were referenced indirectly in a manner similar to that known in the art (e.g., Bax et al., J. Magn. Reson., 67:565-69 (1986)). Carrier frequencies were 4.70 ppm for ¹H, 118 ppm for ¹⁵N, 54 ppm for ¹³C_a, 40 ppm for aliphatic ¹³C, and 174 ppm for ¹³C'. A combination of water flip-back (e.g., Grzesiek et al., J. Am. Chem. Soc., 115:12593-94 (1993)) and WATERGATE (e.g., Piotto et al., <u>J. Biomol. NMR</u>, 2:661-65 (1992)) techniques were used to eliminate

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the water resonance. NMR data were processed using NMRPipe and NMRDraw software from Molecular Simulations, Inc. (San Diego, CA).

Sequence-specific backbone resonance assignments were accomplished using primarily 3-dimensional HNC $_{\alpha}$, HN(CO)C $_{\alpha}$, and C $_{\beta}$ C $_{\alpha}$ (CO)NH data sets. The 13 C' and 1 H $_{\alpha}$, 1 H $_{\beta}$ chemical shifts were determined using HNCO and H $_{\beta}$ H $_{\alpha}$ (CO)NH data sets, respectively. The side chain 1 H and 13 C spin systems were assigned using the 3-dimensional HCCH-TOCSY experiments.

The assigned $^{1}\text{H}^{-15}\text{N}$ HSQC spectrum of HPV-18 E2-DBD is shown in Figure 2. Chemical shift values for all $^{1}\text{H}_{N}$, $^{1}\text{H}_{\alpha}$, $^{13}\text{C}_{\alpha}$, $^{13}\text{C}_{\beta}$, $^{13}\text{C}'$ and $^{15}\text{N}_{\alpha}$ resonances except for the first four residues, the C-terminal five histidine residues, and Glu58 and Thr59 were assigned. Approximately 60% of the side chain ^{1}H and ^{13}C resonances were also assigned. Assigned ^{1}H , ^{13}C , and ^{15}N chemical shifts are listed in Table 1. The locations of secondary structure in the linear amino acid sequence predicted based on $^{13}\text{C}_{\alpha}$ chemical shifts (see Wishart et al., J. Biomol. NMR, 4:171-80 (1994)) are shown in Figure 1 and are consistent with the crystal structures of BPV-1, HPV-16 and HPV-31.

The complete disclosure of all patents, patent applications, and publications, and electronically available material cited herein are incorporated by reference. The foregoing detailed description and examples have been given for clarity of understanding only. No unnecessary limitations are to be understood therefrom. The invention is not limited to the exact details shown and described, for variations obvious to one skilled in the art will be included within the invention defined by the claims.

Table 1: 1 H, 13 C, and 15 N chemical shifts of human papillomavirus E2-DBD. HA, HB, HG, HD, HE, CA, CB, CG, CD, CE refer to H_{α} , H_{β} , H_{γ} , H_{δ} , H_{ϵ} , C_{α} , C_{β} , C_{γ} , C_{δ} , and C_{ϵ} respectively.

5	#Atom	#RES	RES	ATOMS		ppm
	1	4	THR	HA	H	5.01
	2	4	THR	HB	Н	3.91
		4	THR	HG1	Н	0.98
4.0	4	4	THR	HG2	Н	0.98
10	5	4	THR	CA	C	59.95
	6	4	THR	CB	C	67.75
	7	4	THR	CG2	C	19.93
	8	5	THR	Н	Н	9.18
1.5	9	5	THR	С	С	171.68
15	10	5	THR	CA	С	57.48
	11	5	THR	N	N	124.16
	12	6	PRO	HA	H	4.73
	13	6	PRO	CA	C	60.10
20	14	6	PRO	CB	C	29.24
20	15	7	ILE	H	H	8.49
	16	7	ILE	HA	H	5.85
	17	7	ILE	HB	Н	1.82
	18	7	ILE	HG2	Н	0.92
25	19	7 7	ILE	HD1	Н	0.49
25	20 21	7	ILE ILE	C	C	173.65 57.29
	22	7	ILE	CA CB	C	42.10
	23	7	ILE	CG2	C	16.79
	24	7	ILE	CD1	C	12.90
30	25	7	ILE	N	N	115.39
50	26	8	ILE	Н	Н	8.90
	27	8	ILE	HA	H	5.01
	28	8	ILE	НВ	H	1.88
	29	8	ILE	HG2	Н	0.82
35	30	8	ILE	С	С	174.83
	31	8	ILE	CA	С	58.93
	32	8	ILE	CB	C	39.92
	33	8	ILE	CG2	C	15.73
	34	8	ILE	N	N	115.93
40	35	9	HIS	H	Н	8.91
	36	9	HIS	AН	Н	5.68
	37	9	HIS	HB2	Н	2.81
	38	9	HIS	нвз	Н	2.57
15	39	9	HIS	C	C	173.19
45	40	9	HIS	CA	C	51.27
	41	9	HIS	CB	C	32.38
	42	9	HIS	N	N	119.91
	43	10	LEU	H	Н	8.98
50	44 45	10 10	LEU	HA	H H	5.17
50	46	10	LEU	HB2	Н	1.66 0.92
	47	10	LEU LEU	HB3 HG	Н	1.47
	48	10	LEU	HD1	H	0.82
	49	10	LEU	HD2	Н	0.71
55	50	10	LEU	C	C	172.40
	51	10	LEU	CA	Č	50.25
	52	10	LEU	CB	C	40.76
	53	10	LEU	CG	Č	23.68

	54	10	LEU	N	N		122.16
	55 56	11	LYS	H	H		8.76
	56 57	11 11	LYS LYS	HA HB2	H H		5.29 1.65
5	58	11	LYS	HB3	Н		1.44
	59	11	LYS	HG2	Н		1.40
	60 61	11 11	LYS LYS	HG3 HD2	H H		1.21 1.62
	62	11	LYS	HD3	Н		1.62
10	63	11	LYS	HE2	Н		2.70
	64 65	11 11	LYS LYS	HE3 C	H C		2.70 172.59
	66	11	LYS	CA	c		51.76
	67	11	LYS	CB	С		33.58
15	68	11	LYS	CG	С		22.68
	69 70	11 11	LYS LYS	CD CE	C C		27.38 39.54
	71	11	LYS	N	N		120.73
20	72	12	GLY	Н	H		8.30
20	73 74	12 12	GLY GLY	HA2 HA3	H H		4.43 4.19
	75	12	GLY	C	Ç		173.46
	76	12	GLY	CA	C		42.96
25	77	12	GLY	N	N		109.97
25	78 79	13 13	ASP ASP	H HA	H H		8.50 4.59
	80	13	ASP	HB2	Н		2.77
	81	13	ASP	HB3	H		2.61
30	82	13	ASP	C	C		168.61
30	83 84	13 13	ASP ASP	CA CB	C C		52.23 40.03
	85	13	ASP	N	N		120.16
	86	14	ARG	Н	Н		8.61
35	87 88	14 14	ARG ARG	HA HB2	H H	Ψ.	3.58 1.72
33	89	14	ARG	HB3	H		1.68
	90	14	ARG	HG2	Н		1.47
	91	14	ARG	HG3	H		1.47
40	92 93	14 14	ARG ARG	HD2 HD3	H H		3.07 3.02
••	94	14	ARG	C	Ċ		174.68
	95	14	ARG	CA	C		58.64
	96 97	14 14	ARG ARG	CB CG	C C		27.87 26.01
45	98	14	ARG	CD	C		40.85
	99	14	ARG	N	N		122.34
	100	15 15	ASN	H	H		8.64
	101 102	15 15	ASN ASN	HA HB2	H H		4.46 2.87
50	103	15	ASN	нвз	Н		2.76
	104	15	ASN	C	C		176.39
	105 106	15 15	ASN ASN	CA CB	C C		54.42 35.59
	107	15	ASN	N	N		118.46
55	108	16	SER	Н	Н		8.35
	109	16	SER	HA	H		3.86
	110 111	16 16	SER SER	HB2 HB3	H H		4.17 3.63
	112	16	SER	C	C		175.96
60	113	16	SER	CA	C		59.80
	114	16	SER	CB	С		59.96

	115	16	SER	N	N	118.74
	116 117	17 17	LEU LEU	H HA	H H	8.10 3.84
	118	17	LEU	HB2	H	1.64
5	119	17	LEU	HB3	Н	1.17
	120	17	LEU	HD1	H	0.45
	121 122	17 17	LEU LEU	HD2 C	H C	0.38 175.25
	123	17	LEU	CA	Č	55.37
10	124	17	LEU	CB	С	38.75
	125	17	LEU	CD1	С	23.04
	126	17	LEU	CD2	C	19.79
	127 128	17 18	LEU LYS	N H	N H	121.15 7.83
15	129	18	LYS	HA	Н	3.91
	130	18	LYS	HB2	Н	1.97
	131	18	LYS	HB3	Н	1.97
	132	18	LYS	HG2	H	1.39
20	133 134	18 18	LYS LYS	HG3 HD2	H H	1.27 1.70
20	135	18	LYS	HD3	H	1.60
	136	18	LYS	HE2	Н	2.95
	137	18	LYS	HE3	H	2.95
25	138	18	LYS	C	C	175.74
25	139	18	LYS	CA CB	C C	57.85 29.95
	140 141	18 18	LYS LYS	CD	C	27.55
	142	18	LYS	CE	Č	39.77
	143	18	LYS	N	N	120.70
30	144	19	CYS	Н	Н	7.59
	145	19	CYS	HA	H H	4.20 3.02
	146 147	19 19 .	CYS CYS	HB2 HB3	л Н	2.95
	148	19	CYS	C	C	177.01
35	149	19	CYS	CA	С	60.14
	150	19	CYS	CB	C	24.32
	151 152	19 20	CYS LEU	N H	N H	116.91 8.03
	153	20	LEU	HA	Н	4.09
40	154	20	LEU	HB2	Н	1.80
	155	20	LEU	нвз	H	1.54
	156	20	LEU	HD1	H	0.90
	157 158	20 20	LEU LEU	HD2 C	H C	0.82 175.16
45	159	20	LEU	CA	Č	55.39
	160	20	LEU	CB	С	39.82
	161	20	LEU	CD1	C	21.58
	162	20 20	LEU	CD2	C N	25.17 121.40
50	163 164	21	LEU ARG	N H	Н	8.58
	165	21	ARG	НA	H	3.61
	166	21	ARG	HB2	H	1.95
	167	21	ARG	C	C	175.45
55	168 169	21 21	ARG ARG	CA CB	C C	58.16 27.32
))	169 170	21	ARG ARG	N N	N	118.96
	171	22	TYR	Н	Н	7.43
	172	22	TYR	HA	Н	3.91
<i>(</i> 0	173	22	TYR	C	C	175.54
60	174 175	22	TYR TVD	CA	C C	59.04 35.58
	175	22	TYR	CB	C	55.58

	176 177 178 179	22 23 23 23	TYR ARG ARG	N H HA	N H H	116.61 7.88 4.04
5	180 181 182 183	23 23 23 23 23	ARG ARG ARG ARG ARG	HB2 HB3 HG2 HG3 HD2	H H H H H	2.04 2.04 1.70 1.70 3.26
10	184 185 186 187 188	23 23 23 23 23	ARG ARG ARG ARG ARG	HD3 C CA CB CG	H C C C	3.26 176.67 57.11 28.01 25.77
15	189 190 191 192 193	23 23 24 24 24	ARG ARG LEU LEU LEU	CD N H HA HB2	C N H H	41.55 119.89 8.59 4.18 1.89
20	194 195 196 197 198	24 24 24 24 24	LEU LEU LEU LEU	HB3 HD1 HD2 C CA	Н Н С С	1.46 0.80 0.60 177.05 55.00
25	199 200 201 202 203	24 24 24 24 25	LEU LEU LEU ARG	CB CD1 CD2 N H	C C N H	38.81 21.32 22.99 117.28 7.75
30	204 205 206 207 208	25 25 25 25 25	ARG ARG ARG ARG	HA HB2 HB3 HG2 HG3	H H H H	4.26 1.91 1.91 1.82 1.82
35	209 210 211 212 213	25 25 25 25 25	ARG ARG ARG ARG ARG	HD2 HD3 C CA CB	н С С С	3.11 3.11 177.46 56.71 27.46
40	214 215 216 217 218	25 25 25 26 26	ARG ARG ARG LYS LYS	CG CD N H HA	C N H	25.14 41.30 120.30 7.28 4.17
45	219 220 221 222 223	26 26 26 26 26	LYS LYS LYS LYS	HB2 HB3 HG2 HG3 HD2	H H H H	1.60 1.60 1.22 1.22 1.57
50	224 225 226 227 228	26 26 26 26 26	LYS LYS LYS LYS	HD3 HE2 HE3 C CA	Н Н С С	1.57 2.86 2.88 175.55 54.84
55	229 230 231 232 233	26 26 26 26 26	LYS LYS LYS LYS	CB CG CD CE N	CCCN	29.70 22.19 26.73 39.22 115.77
60	234 235 236	27 27 27	HIS HIS HIS	H HA HB2	H H H	7.82 5.01 3.40

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353 40 TRP N N 120.03 354 41 THR H H 8.67 355 41 THR HA H 4.42 356 41 THR HB H 3.92 60 357 41 THR HG2 H 0.99							
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60 357 41 THR HG2 H 0.99							
	60						
							175.17

	359	41	THR	CA	С	62.27
	360	41	THR	CB	С	67.99
	361	41	THR	CG2	С	20.38
_	362	41	THR	N	N	115.31
5	363	42	GLY	Н	H	9.77
	364	42	GLY	HA2	H	4.03
	365	42	GLY	HA3	H	4.03
	366 367	42 42	GLY	C CA	C C	173.88 43.28
10	368	42	${ t GLY}$	N N	N	114.16
10	369	43	ALA	H	H	8.31
	370	43	ALA	HA	H	4.32
	371	43	ALA	HB	H	1.39
	372	43	ALA	C	Ċ	172.26
15	373	43	ALA	CA	Č	50.72
	374	43	ALA	CB	Č	16.84
	375	43	ALA	N	N	123.70
	376	44	GLY	Н	Н	8.42
	377	44	GLY	HA2	Н	4.10
20	378	44	GLY	HA3	Н	3.91
	379	44	GLY	С	С	176.29
	380	44	GLY	CA	С	43.25
	381	44	GLY	N	N	108.16
25	382	45	ASN	HA	Н	4.75
25	383	45	ASN	HB2	Н	2.93
	384	45	ASN	HB3	H	2.75
	385	45	ASN	C	C	172.12
	386	45	ASN	CA	C	50.98
30	387 388	45 45	ASN	CB	C	37.51
30	389	45 46	ASN GLU	N H	N H	117.19 8.81
	390	46	GLU	нA	Н	3.98
	391	46	GLU	HB2	H	1.93
	392	46	GLU	HB3	Н	1.87
35	393	46	GLU	HG2	H	2.14
	394	46	GLU	HG3	Н	2.14
	395	46	GLU	C	С	173.36
	396	46	GLU	CA	С	55.97
	397	46	GLU	CB	С	27.17
40	398	46	GLU	CG	С	33.95
	399	46	GLU	N	N	119.81
	400	47	LYS	H	Н	8.17
	401	47	LYS	HA	Н	4.19
15	402	47	LYS	HB2	H	1.94
45	403	47	LYS	HB3	H	1.76
	404 405	47 47	LYS	HG2	H	1.40
	405	47	LYS LYS	HG3 HD2	H H	1.33
	407	47	LYS	HD3	H	1.60 1.60
50	408	47	LYS	HE2	Н	2.94
• •	409	47	LYS	HE3	H	2.94
	410	47	LYS	C	C	174.43
	411	47	LYS	CA	Č	54.79
	412	47	LYS	CB	C	30.57
55	413	47	LYS	CG	С	22.93
	414	47	LYS	CD	С	26.73
	415	47	LYS	CE	С	39.80
	416	47	LYS	N	N	117.28
~ ^	417	48	THR	Н	H	7.49
60	418	48	THR	HA	Н	4.37
	419	48	THR	HB	Н	3.99

	420	48	THR	HG1	Н	1.05
	421	48	THR	HG2	H C	1.05 174.80
	422 423	48 48	THR THR	C CA	C	59.28
5	424	48	THR	CB	Č	68.23
•	425	48	THR	CG2	С	19.72
	426	48	THR	N	N	113.55
	427	49	GLY	H	Н	8.64
10	428	49	GLY	HA2	Н	4.28
10	429	49	GLY	HA3	H	3.05
	430 431	49 49	GLY GLY	C CA	C C	171.67 42.01
	431	49	GLY	N	N	111.32
	433	50	ILE	H	Н	8.29
15	434	50	ILE	HA	Н	4.53
	435	50	ILE	HB	H	-1.31
	436	50	ILE	HG2	H	-0.31
	437	50	ILE	C	C	168.12
20	438	50	ILE	CA	C	57.68 37.82
20	439 440	50 50	ILE ILE	CB N	C N	119.88
	441	51	LEU	Н	Н	8.39
	442	51	LEU	нA	H	4.30
	443	51	LEU	HB2	H	1.44
25	444	51	LEU	HB3	H	1.24
	445	51	LEU	HG	Н	1.44
	446	51	LEU	HD1	H	0.67
	447	51	LEU	C	C	171.45
30	448 449	51 51	LEU LEU	CA CB	C C	51.06 44.03
50	450	51	LEU	CG	Ċ	24.41
	451	51	LEU	CD1	Č	23.46
	452	51	LEU	N	N	120.99
	453	52	THR	Н	Н	. 8.89
35	454	52	THR	HA	H	5.22
	455	52	THR	HB	Н	3.52
	456 457	52 52	THR THR	HG2 C	H C	1.30 173.14
	458	52	THR	CA	C	59.30
40	459	52	THR	CB	Č	72.25
	460	52	THR	CG2	С	22.71
	461	52	THR	N	N	120.58
	462	53	VAL	H	Н	8.97
45	463	53	VAL	HA	H	4.71
43	464 465	53 53	VAL VAL	HB HG1	H H	1.65 0.43
	466	53	VAL	HG2	H	0.16
	467	53	VAL	C	C	170.60
	468	53	VAL	CA	C	58.06
50	469	53	VAL	СВ	C	31.00
	470	53	VAL	CG1	С	18.20
	471	53	VAL	CG2	C	20.37
	472	53 54	VAL	N	N	127.66 8.63
55	473 474	54 54	THR THR	H HA	H H	5.00
55	475	54	THR	HB	H	3.87
	476	54	THR	HG2	Н	1.03
	477	54	THR	С	С	172.93
	478	54	THR	CA	С	56.41
60	479	54	THR	CB	С	68.61
	480	54	THR	CG2	С	19.60

	481	54	THR	N	N	114.36
	482	55 55	TYR	H	Н	7.26 4.61
	483	55 55	TYR TYR	HA HB2	H H	3.55
5	484 485	55	TYR	HB3	Н	3.55
,	486	55	TYR	C	C	171.06
	487	55	TYR	CA	Č	55.21
	488	55	TYR	CB	Č	40.88
	489	55	TYR	N	N	113.74
10	490	56	HIS	H	H	9.34
	491	56	HIS	HA	Н	4.42
	492	56	HIS	HB2	Н	3.08
	493	56	HIS	нв3	Н	2.81
	494	56	HIS	С	С	173.18
15	495	56	HIS	CA	С	56.49
	496	56	HIS	CB	С	29.81
	497	56	HIS	N	N	118.21
	498	57	SER	H	Н	7.34
	499	57	SER	C	С	173.49
20	500	57	SER	CA	С	54.41
	501	57	SER	N	N	105.78
	502	59	THR	HА	Н	3.91
	503	59	THR	HB	Н	4.07
~~	504	59	THR	HG2	H	1.20
25	505	59	THR	CA	C	64.19
	506	59	THR	CB	C	66.34
	507	59	THR	CG2	C	18.99
	508	60	GLN	H	H	8.02
20	509	60	GLN	HA	H	4.06
30	510	60 60	GLN	HB2	H	2.09
	511	60	GLN	HB3	H	3.26
	512 513	60 60 ·	GLN GLN	HG2 HG3	H H	3.26
	514	60 .	GLN	C	C	174.20
35	515	60	GLN	CA	C	56.90
55	516	60	GLN	CB	Č	27.27
	517	60	GLN	CG	Č	41.55
	518	60	GLN	N	N	123.81
	519	61	ARG	Н	Н	7.31
40	520	61	ARG	нА	Н	2.99
	521	61	ARG	HB2	Н	1.70
	522	61	ARG	нвз	H	1.70
	523	61	ARG	С	С	175.22
	524	61	ARG	CA	C	57.25
45	525	61	ARG	CB	C	27.77
	526	61	ARG	N	N	119.25
	527	62	THR	H	Η	8.47
	528	62	THR	HA	Н	3.71
	529	62	THR	HB	H	4.21
50	530	62	THR	HG2	H	1.16
	531	62	THR	C	C	174.94
	532	62	THR	CA	С	64.67
	533	62	THR	CB	C	66.46
<i>5 </i>	534	62	THR	CG2	C	19.65
55	535	62	THR	N	N	117.57
	536	63	LYS	H	Н	7.88
	537	63	LYS	HA	Н	4.05
	538	63	LYS	HB2	Н	1.90
60	539	63	LYS	HB3	Н	1.90 1.29
60	540	63	LYS	HG2 HG3	H H	1.29
	541	63	LYS	дСЭ	п	1.42

543 63 LYS HD3 H 1.59 544 63 LYS HE2 H 2.84 545 63 LYS CC 173.47 546 63 LYS CC C 173.47 547 63 LYS CB C 29.34 549 63 LYS CD C 22.63 550 63 LYS CD C 26.76 10 551 63 LYS CD C 26.76 550 63 LYS N N 121.56 551 63 LYS N N 121.56 553 64 PHE HB H 3.75 555 64 PHE HB H 3.75 557 64 PHE CB C 177.53 556 64 PHE CC C 177.53 556 <		542	63	LYS	HD2	Н		1.59
544 63 LYS HE2 H 2.84 545 646 63 LYS C C 173.47 547 63 LYS CA C 57.28 548 63 LYS CB C 29.34 550 63 LYS CD C 226.76 10 551 63 LYS CD C 226.76 10 551 63 LYS CD C 226.76 10 551 63 LYS CD C 226.76 10 553 64 PHE HA H 3.94 553 64 PHE HA H 3.75 15 556 64 PHE C C 177.53 557 64 PHE C C 177.53 558 64 PHE N N 122.19 560 65								
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	605	69	ALA	CB	C	15.99
	606	69	ALA	N	N	129.17
5	607	70	ILE	Н	Н	8.40
	608	70	ILE	С	С	174.04
	609	70	ILE	CA	C	54.26
	610 611	70	ILE	N	N	125.89 4.43
10	612	71 71	PRO PRO	HA HB3	H H	1.92
10	613	71	PRO	HG2	Н	3.83
	614	71	PRO	HG3	Н	3.35
	615	71	PRO	CA	C	60.85
	616	71	PRO	CB	С	30.38
15	617	71	PRO	CG	С	25.23
	618	72	ASP	H	Н	8.56
	619	72	ASP	HA	Н	4.19
	620 621	72 72	ASP ASP	HB2 HB3	H H	2.65 2.65
20	622	72 72	ASP	С	C	174.61
	623	72	ASP	CA	Č	53.85
	624	72	ASP	CB	Ċ	38.07
	625	72	ASP	N	N	120.03
	626	73	SER	Н	Н	7.48
25	627	73	SER	HA	Н	4.26
	628	73 73	SER	HB2	H	4.07
	629 630	73 73	SER	НВЗ С	H C	3.83 173.98
	631	73 73	SER SER	CA	C	55.90
30	632	73	SER	CB	Č	60.58
	633	73	SER	N	N	109.69
	634	74	VAL	H	Н	7.83
	635	74	VAL	HA	Н	4.45
25	636	74	VAL	HB	H	1.99
35	637	74	VAL	HG1	H	0.66
	638 639	74 74	VAL VAL	HG2 C	H C	0.62 171.92
	640	74	VAL	CA	Ċ	59.08
	641	74	VAL	CB	Č	30.98
40	642	74	VAL	CG1	C	20.02
	643	74	VAL	CG2	С	20.02
	644	74	VAL	N	N	125.42
	645	75 75	GLN	H	H	8.94
45	646 647	75 75	GLN	HA HB2	H H	4.45 2.03
7,7	648	75 75	GLN GLN	HB3	Н	1.90
	649	75	GLN	HG2	Н	2.43
	650	75	GLN	HG3	Н	2.23
	651	75	GLN	C	С	172.04
50	652	75	GLN	CA	С	53.00
	653	75 75	GLN	CB	C	28.74
	654	75	GLN	CG	C	32.19
	655 656	75 76	GLN ILE	N H	N H	125.65 8.83
55	657	76	ILE	n HA	H	4.63
	658	76	ILE	HB	H	1.88
	659	76	ILE	HG2	Н	0.67
	660	76	ILE	С	С	172.76
<i>(</i> 0	661	76	ILE	CA	C	58.71
60	662	76	ILE	CB	C	37.76
	663	76	ILE	CG2	С	15.81

	664	76	ILE	N	N	122.43
	665	77	LEU	Н	H	9.07
	666	77	LEU	HA	H	5.04
5	667	77	LEU	HB2	H	1.65 1.30
)	668 669	77 77	LEU LEU	HB3 HG	H H	1.43
	670	77	LEU	HD1	Н	0.74
	671	77	LEU	HD2	H	0.60
	672	77	LEU	С	С	172.98
10	673	77	LEU	CA	С	51.54
	674	77	LEU	CB	С	41.98
	675	77	LEU	CG	С	25.94
	676	77	LEU	CD1	C	22.69
15	677	77	LEU	CD2	C	22.12
15	678	77	LEU	N	N	128.16 8.87
	679 680	78 78	VAL VAL	H HA	H H	4.38
	681	78	VAL	HB	H	1.55
	682	78	VAL	HG1	Н	0.71
20	683	78	VAL	HG2	Н	0.71
	684	78	VAL	С	С	173.14
	685	78	VAL	CA	С	58.45
	686	78	JAV	CB	С	32.33
25	687	78	VAL	CG1	C	19.09
25	688	78	VAL	CG2	C	19.09
	689	78 70	VAL	N	N	121.05
	690 691	79 79	GLY	H HA2	H H	7.86 5.08
	692	79 79	GLY	HA3	Н	4.08
30	693	79	GLY	C	C	172.86
	694	79	GLY	CA	Č	44.62
	695	79	GLY	N	N	111.73
	696	80	TYR	Н	Н	8.54
	697	80	TYR	HA	Н	5.37
35	698	80	TYR	HB2	Н	2.99
	699	80	TYR	HB3	H	2.61
	700 701	80 80	TYR	C CA	C C	169.75 5 4. 23
	701	80	TYR TYR	CB	C	40.30
40	702	80	TYR	N	N	119.24
••	704	81	MET	Н	Н	8.60
	705	81	MET	HA	Н	5.35
	706	81	MET	HB2	Н	1.94
	707	81	MET	HB3	Н	1.94
45	708	81	MET	HG2	Н	2.55
	709	81	MET	HG3	H	2.50
	710	81	MET	C	C	171.31
	711 712	81 81	MET MET	CA CB	C C	51.86 34.66
50	713	81	MET	CG	C	29.09
50	714	81	MET	Ŋ	N	117.15
	715	82	THR	Н	Н	8.53
	716	82	THR	HA	Н	4.98
	717	82	THR	HB	Н	3.51
55	718	82	THR	HG2	Н	1.06
	719	82	THR	C	C	172.03
	720	82	THR	CA	C	59.38
	721	82	THR	CB	C	68.52
60	722	82	THR	CG2	C	19.60
UU	723 72 4	82 83	THR MET	N H	N H	122.12 8.25
	127	55	7.771 T	11	**	0.23

	725	83	MET	HA	H	5.19
	726	83	MET	С	С	170.95
	727	83	MET	CA	С	51.06
	728	83	MET	CB	С	33.27
5	729	83	MET	N	N	122.01
_	730	84	HIS	H	Н	8.90
	731	84	HIS	С	С	173.02
	732	84	HIS	CA	С	53.04
	733	84	HIS	N	N	118.65
10						